Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Tetrakis(4-cyanopyridine)palladium(II) bis(trifluoromethanesulfonate)

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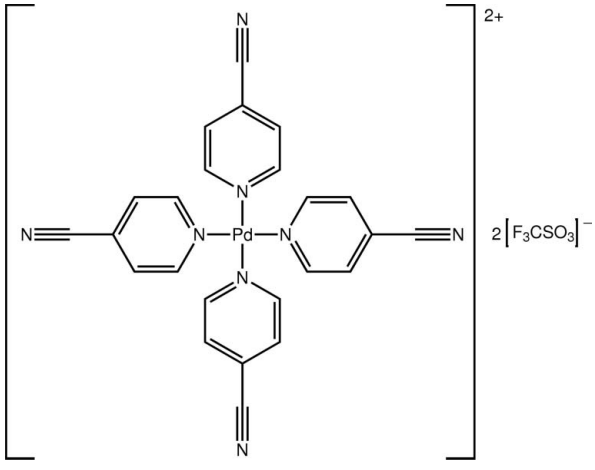
Received 9 July 2010; accepted 13 July 2010

Key indicators: single-crystal X-ray study; T = 153 K; mean σ(C–C) = 0.008 Å; R factor = 0.048; wR factor = 0.128; data-to-parameter ratio = 12.4.

The title salt, $[Pd(C_6H_4N_2)_4](CF_3SO_3)_2$, comprises Pd(4-cyanopyridine)$_4$ dications balanced by two trifluoromethanesulfonate anions. The Pd^{II} atom lies in a square-planar geometry defined by four N atoms which form equivalent Pd—N interactions. The 4-cyanopyridine ligands are twisted out of the N_4 plane, forming dihedral angles ranging from 66.5 (2) to 89.9 (2)°. In the crystal packing, columns of edge-to-edge dications define channels in which reside the anions. A range of C—H···N and C—H···O hydrogen-bonding interactions stabilizes the crystal packing.

Related literature

For related palladium(II) complexes with 4-cyanopyridine, see: Kopylovich *et al.* (2009); Lang *et al.* (2006); Taher *et al.* (2006).



Experimental

Crystal data

$[Pd(C_6H_4N_2)_4](CF_3O_3S)_2$
M_r = 820.99
Monoclinic, $P2_1/c$
a = 18.550 (4) Å
b = 9.2993 (19) Å
c = 20.688 (4) Å
β = 114.55 (3)°
V = 3246.1 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.79 mm^{-1}
T = 153 K
0.20 × 0.20 × 0.20 mm

Data collection

Rigaku AFC12/SATURN724 diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.829, T_{max} = 1.000
12799 measured reflections
5478 independent reflections
5000 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.128
S = 1.14
5478 reflections
442 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.05 e Å^{-3}
$\Delta\rho_{min}$ = −0.74 e Å^{-3}

Table 1
Selected bond lengths (Å).

Pd—N1	2.027 (4)	Pd—N5	2.029 (4)
Pd—N3	2.031 (4)	Pd—N7	2.027 (4)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···N8^{i}	0.95	2.56	3.489 (8)	166
C5—H5···O2	0.95	2.44	3.159 (6)	132
C7—H7···O5^{ii}	0.95	2.52	3.202 (6)	129
C8—H8···N6^{iii}	0.95	2.53	3.441 (8)	160
C13—H13···O5^{ii}	0.95	2.33	3.134 (7)	141
C16—H16···N6^{iv}	0.95	2.61	3.403 (8)	142
C22—H22···O3^{v}	0.95	2.52	3.170 (7)	126
C23—H23···O2	0.95	2.34	3.163 (7)	145

Symmetry codes: (i) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$; (ii) $x, y-1, z$; (iii) $-x, y-\frac{1}{2}, -z+\frac{3}{2}$; (iv) $-x, -y+1, -z+1$; (v) $-x+1, y-\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: *CrystalClear* (Molecular Structure Corporation & Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

This research was supported by National Institutes of Health grant No. SO6–08194. The authors also appreciate the support of the Chemistry Department at The University of the Incarnate Word.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: EZ2223).

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supporting information

Acta Cryst. (2010). E**66**, m957–m958 [https://doi.org/10.1107/S1600536810027704]

Tetrakis(4-cyanopyridine)palladium(II) bis(trifluoromethanesulfonate)

Rafael A. Adrian, David M. Gonzalez, Edward R. T. Tiekink and Judith A. Walmsley

S1. Comment

While studying the palladium-catalyzed hydration of nitriles, we sought to crystallize palladium(II) complexes with 4-cyanopyridine, similar to those created by Kopylovich *et al.* (2009), Lang *et al.* (2006) and Taher *et al.* (2006). The resulting yellow crystals that formed, (I), were found not to contain any ethylenediamine, but contained a palladium(II) center where the inner coordination sphere is occupied by 4-cyanopyridine ligands.

The molecular structure of (I) comprises a Pd(4-cyanopyridine)$_4$ dication, Fig. 1, and two trifluoromethanesulfonate anions. The palladium atom lies in a square planar geometry defined by four pyridine-N atoms which form experimentally equivalent Pd–N bond distances, Table 1. The palladium atom lies in the least-squares plane through the N_4 donor set with the r.m.s. deviation for the PdN_4 atoms being 0.021 Å. For steric reasons, each of the 4-cyanopyridine molecules is twisted with respect to the N_4 plane, forming dihedral angles with it of 72.21 (19), 66.5 (2), 80.1 (2), and 89.9 (2) ° for the N1-, N3-, N5-, and N7-pyridine rings, respectively.

In the crystal packing, molecules self-assemble into layers in the *ab* plane *via* *C–H*···N_{cyano} and C–H···O interactions, Table 2. The resulting 2-D array, Fig. 2, can be described as comprising rows of edge-to-edge complex dications that define channels in which reside the anions, Fig. 3.

S2. Experimental

Pd(ethylenediamine)(trifluoromethanesulfonate)$_2$ was prepared by adding solid Ag(trifluoromethanesulfonate) to an aqueous solution of Pd(ethylenediamine)Cl_2 (0.050 g, 0.21 mmol). After stirring for 1 h, the mixture was filtered to remove AgCl. 4-Cyanopyridine (0.090 g, 0.85 mmol) was added to the Pd(ethylenediamine)(trifluoromethanesulfonate)$_2$ solution and heated at 323 K for 2 h. The solution was then allowed to evaporate at room temperature, yielding a yellow solid. X-ray diffraction quality crystals were obtained by vapor diffusion of diethyl ether over a CH_3CN solution of the title complex, (I). (0.026 g, 15% yield). IR (cm^{-1}, solid): *ν*(═CH) 3112 (w), 3083(w), 3022(w); *ν*(CN) 2244 (w); *ν*s(CF_3) 1220 (*s*), *ν*s(SO_3) 1028 (*s*). *M*.pt.: 498 K (dec.) with melting at 523 K.

S3. Refinement

The H-atoms were included in the refinement in the riding model approximation (C–H = 0.95 Å) with U_{iso}(H) set to 1.2U_{eq}(carrier atom). The maximum and minimum residual electron density peaks of 1.05 and 0.74 e Å^{-3}, respectively, were located 0.71 Å and 0.63 Å from the C11 and S1 atoms, respectively.

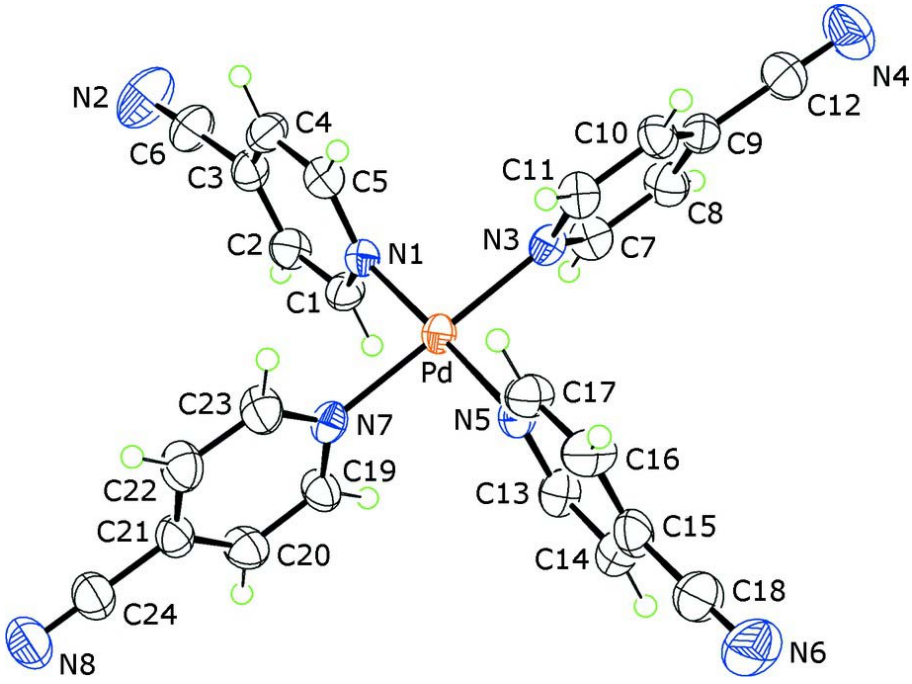

Figure 1

Molecular structure of the cation in (I) showing atom-labelling scheme and displacement ellipsoids at the 50% probability level.

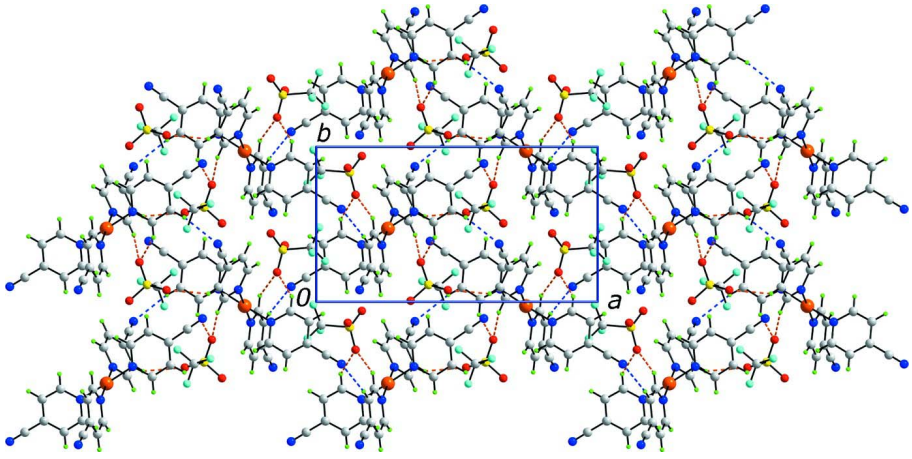

Figure 2

Supramolecular 2-D array (I) mediated by C–H···N and C–H···O contacts (blue and orange dashed lines, respectively). Colour code: Pd, orange; S, yellow; O, red; N, blue; C, grey; H, green.

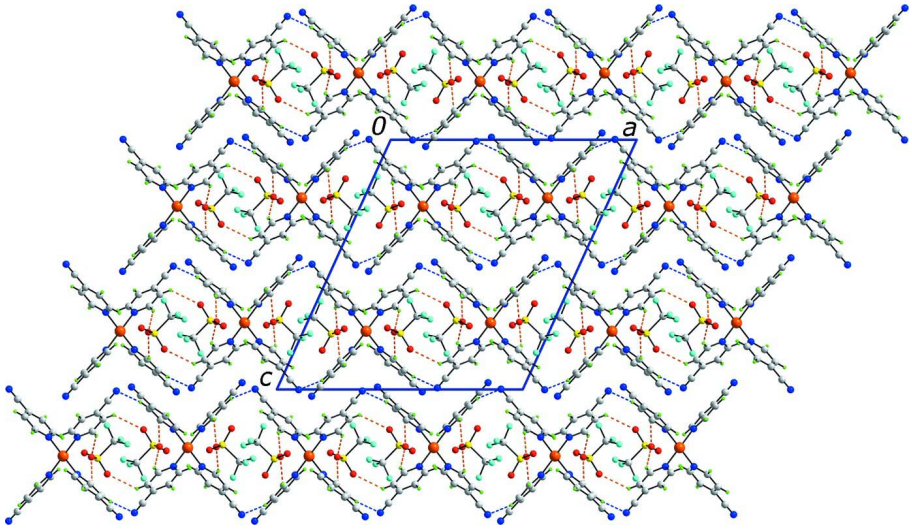

Figure 3

Stacking of layers in (I), highlighting the formation of channels by the dications in which reside the anions. The C–H···N and C–H···O contacts are shown as blue and orange dashed lines, respectively. Colour code: Pd, orange; S, yellow; O, red; N, blue; C, grey; H, green.

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Crystal data

$[Pd(C_6H_4N_2)_4](CF_3O_3S)_2$
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Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 18.550$ (4) Å
$b = 9.2993$ (19) Å
$c = 20.688$ (4) Å
$\beta = 114.55$ (3)°
$V = 3246.1$ (14) Å^3
$Z = 4$
$F(000) = 1632$
$D_x = 1.680$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4545 reflections
$\theta = 2.4$–26.7°
$\mu = 0.79$ mm^{-1}
$T = 153$ K
Block, pale-yellow
0.20 × 0.20 × 0.20 mm

Data collection

Rigaku AFC12K/SATURN724 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.829$, $T_{max} = 1.000$
12799 measured reflections
5478 independent reflections
5000 reflections with $I > 2\sigma(I)$
$R_{int} = 0.035$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.4°$
$h = -22 \rightarrow 20$
$k = -9 \rightarrow 11$
$l = -24 \rightarrow 22$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.128$
$S = 1.14$
5478 reflections
442 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0534P)^2 + 6.3187P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.05$ e Å^{-3}
$\Delta\rho_{min} = -0.74$ e Å^{-3}

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Pd	0.254695 (18)	0.02757 (4)	0.766848 (17)	0.02851 (14)
S1	0.39867 (7)	0.39076 (14)	0.77597 (7)	0.0421 (3)
S2	0.11861 (7)	0.66442 (14)	0.77812 (7)	0.0384 (3)
F1	0.3763 (3)	0.3677 (5)	0.6440 (2)	0.0951 (14)
F2	0.4595 (3)	0.5294 (4)	0.7007 (3)	0.0944 (14)
F3	0.4938 (3)	0.3095 (5)	0.7191 (2)	0.0874 (13)
F4	−0.03138 (19)	0.7372 (4)	0.7237 (2)	0.0733 (10)
F5	−0.0103 (2)	0.5195 (4)	0.7061 (3)	0.0954 (15)
F6	0.0144 (2)	0.6830 (5)	0.64715 (19)	0.0856 (12)
O1	0.3355 (2)	0.4938 (4)	0.7542 (2)	0.0559 (10)
O2	0.3714 (2)	0.2450 (4)	0.7711 (2)	0.0571 (10)
O3	0.4674 (2)	0.4248 (5)	0.8390 (2)	0.0701 (13)
O4	0.1119 (2)	0.6364 (5)	0.8435 (2)	0.0661 (12)
O5	0.1394 (2)	0.8100 (4)	0.7697 (2)	0.0499 (9)
O6	0.1616 (2)	0.5589 (4)	0.7574 (2)	0.0545 (10)
N1	0.3470 (2)	−0.0809 (4)	0.84066 (18)	0.0300 (8)
N2	0.5954 (3)	−0.3914 (7)	1.0098 (3)	0.0771 (17)
N3	0.2329 (2)	0.1341 (4)	0.84253 (19)	0.0306 (8)
N4	0.1540 (3)	0.4235 (6)	1.0271 (3)	0.0672 (14)
N5	0.1614 (2)	0.1304 (4)	0.69095 (19)	0.0316 (8)
N6	−0.0892 (3)	0.4022 (6)	0.4987 (3)	0.0653 (14)
N7	0.2771 (2)	−0.0774 (4)	0.69126 (19)	0.0318 (8)
N8	0.3503 (3)	−0.3732 (6)	0.5062 (2)	0.0570 (12)
C1	0.3401 (3)	−0.2230 (5)	0.8488 (2)	0.0354 (10)
H1	0.2905	−0.2682	0.8230	0.042*
C2	0.4029 (3)	−0.3051 (5)	0.8936 (2)	0.0392 (11)
H2	0.3966	−0.4052	0.8988	0.047*
C3	0.4752 (3)	−0.2391 (6)	0.9307 (2)	0.0380 (11)
C4	0.4820 (3)	−0.0920 (6)	0.9233 (2)	0.0405 (11)
H4	0.5310	−0.0444	0.9490	0.049*

C5	0.4169 (3)	−0.0165 (5)	0.8782 (2)	0.0349 (10)
H5	0.4215	0.0843	0.8735	0.042*
C6	0.5424 (3)	−0.3230 (6)	0.9757 (3)	0.0501 (13)
C7	0.2062 (3)	0.0623 (6)	0.8847 (2)	0.0399 (11)
H7	0.2007	−0.0392	0.8804	0.048*
C8	0.1865 (3)	0.1317 (6)	0.9340 (3)	0.0437 (12)
H8	0.1679	0.0793	0.9634	0.052*
C9	0.1945 (3)	0.2796 (5)	0.9396 (2)	0.0360 (11)
C10	0.2225 (3)	0.3537 (5)	0.8974 (2)	0.0374 (11)
H10	0.2288	0.4552	0.9011	0.045*
C11	0.2414 (3)	0.2758 (5)	0.8491 (2)	0.0364 (11)
H11	0.2610	0.3258	0.8197	0.044*
C12	0.1719 (3)	0.3602 (6)	0.9892 (3)	0.0493 (13)
C13	0.0912 (3)	0.0632 (6)	0.6598 (3)	0.0390 (11)
H13	0.0869	−0.0332	0.6731	0.047*
C14	0.0258 (3)	0.1282 (6)	0.6098 (3)	0.0419 (12)
H14	−0.0230	0.0779	0.5882	0.050*
C15	0.0324 (3)	0.2699 (6)	0.5912 (2)	0.0424 (12)
C16	0.1042 (3)	0.3394 (6)	0.6227 (3)	0.0460 (12)
H16	0.1096	0.4360	0.6105	0.055*
C17	0.1682 (3)	0.2669 (5)	0.6723 (2)	0.0406 (11)
H17	0.2179	0.3142	0.6938	0.049*
C18	−0.0355 (3)	0.3426 (6)	0.5394 (3)	0.0514 (14)
C19	0.2442 (3)	−0.2063 (5)	0.6675 (2)	0.0383 (11)
H19	0.2079	−0.2450	0.6845	0.046*
C20	0.2615 (3)	−0.2836 (6)	0.6192 (3)	0.0425 (12)
H20	0.2377	−0.3746	0.6028	0.051*
C21	0.3145 (3)	−0.2260 (5)	0.5948 (2)	0.0370 (11)
C22	0.3479 (3)	−0.0935 (6)	0.6189 (3)	0.0453 (12)
H22	0.3839	−0.0519	0.6024	0.054*
C23	0.3278 (3)	−0.0227 (6)	0.6675 (3)	0.0426 (12)
H23	0.3509	0.0684	0.6847	0.051*
C24	0.3344 (3)	−0.3078 (6)	0.5450 (3)	0.0462 (13)
C25	0.4345 (4)	0.4002 (7)	0.7071 (4)	0.0596 (16)
C26	0.0176 (3)	0.6496 (6)	0.7111 (3)	0.0548 (14)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pd	0.0277 (2)	0.0264 (2)	0.0324 (2)	0.00416 (13)	0.01340 (16)	0.00318 (13)
S1	0.0410 (7)	0.0374 (7)	0.0541 (7)	−0.0029 (6)	0.0259 (6)	−0.0035 (6)
S2	0.0339 (6)	0.0349 (7)	0.0495 (7)	0.0020 (5)	0.0202 (5)	0.0073 (5)
F1	0.120 (4)	0.117 (4)	0.054 (2)	−0.012 (3)	0.042 (2)	−0.002 (2)
F2	0.125 (4)	0.060 (3)	0.141 (4)	−0.020 (2)	0.098 (3)	0.008 (2)
F3	0.105 (3)	0.089 (3)	0.106 (3)	0.034 (3)	0.081 (3)	0.019 (2)
F4	0.0419 (18)	0.072 (3)	0.097 (3)	0.0145 (18)	0.0206 (18)	−0.004 (2)
F5	0.059 (2)	0.055 (2)	0.155 (4)	−0.0209 (19)	0.027 (3)	−0.007 (2)
F6	0.069 (2)	0.119 (4)	0.053 (2)	−0.011 (2)	0.0098 (18)	−0.002 (2)

O1	0.051 (2)	0.045 (2)	0.075 (3)	0.0109 (18)	0.029 (2)	−0.0001 (19)
O2	0.072 (3)	0.038 (2)	0.078 (3)	−0.0120 (19)	0.048 (2)	0.0012 (19)
O3	0.045 (2)	0.097 (4)	0.063 (3)	−0.002 (2)	0.017 (2)	−0.026 (3)
O4	0.060 (2)	0.092 (3)	0.060 (2)	0.019 (2)	0.038 (2)	0.026 (2)
O5	0.041 (2)	0.038 (2)	0.066 (2)	−0.0062 (16)	0.0177 (18)	0.0011 (17)
O6	0.048 (2)	0.048 (2)	0.074 (3)	0.0121 (18)	0.032 (2)	0.002 (2)
N1	0.0284 (19)	0.031 (2)	0.0310 (19)	0.0028 (16)	0.0124 (16)	−0.0009 (16)
N2	0.047 (3)	0.080 (4)	0.086 (4)	0.017 (3)	0.009 (3)	0.031 (3)
N3	0.0274 (18)	0.029 (2)	0.0354 (19)	0.0015 (16)	0.0130 (16)	0.0055 (16)
N4	0.080 (4)	0.079 (4)	0.057 (3)	0.001 (3)	0.042 (3)	−0.014 (3)
N5	0.032 (2)	0.029 (2)	0.0340 (19)	0.0043 (16)	0.0146 (16)	0.0028 (16)
N6	0.058 (3)	0.064 (3)	0.058 (3)	0.018 (3)	0.007 (3)	0.010 (3)
N7	0.0269 (19)	0.033 (2)	0.0353 (19)	0.0051 (16)	0.0123 (16)	0.0062 (17)
N8	0.063 (3)	0.065 (3)	0.049 (3)	0.010 (3)	0.030 (2)	−0.005 (2)
C1	0.032 (2)	0.031 (3)	0.041 (2)	−0.001 (2)	0.013 (2)	−0.002 (2)
C2	0.043 (3)	0.031 (3)	0.039 (3)	0.007 (2)	0.013 (2)	0.002 (2)
C3	0.035 (3)	0.045 (3)	0.032 (2)	0.011 (2)	0.012 (2)	0.005 (2)
C4	0.030 (2)	0.051 (3)	0.038 (3)	−0.003 (2)	0.011 (2)	0.000 (2)
C5	0.039 (3)	0.032 (3)	0.036 (2)	−0.001 (2)	0.018 (2)	0.002 (2)
C6	0.037 (3)	0.055 (4)	0.051 (3)	0.008 (3)	0.011 (2)	0.009 (3)
C7	0.043 (3)	0.038 (3)	0.040 (3)	−0.001 (2)	0.019 (2)	0.004 (2)
C8	0.049 (3)	0.048 (3)	0.040 (3)	−0.005 (2)	0.025 (2)	0.000 (2)
C9	0.032 (2)	0.046 (3)	0.029 (2)	0.004 (2)	0.0117 (19)	0.000 (2)
C10	0.040 (3)	0.033 (3)	0.038 (2)	0.006 (2)	0.016 (2)	−0.001 (2)
C11	0.041 (3)	0.032 (3)	0.041 (3)	0.001 (2)	0.021 (2)	0.006 (2)
C12	0.052 (3)	0.057 (4)	0.043 (3)	0.001 (3)	0.024 (3)	−0.003 (3)
C13	0.039 (3)	0.038 (3)	0.043 (3)	0.005 (2)	0.019 (2)	0.008 (2)
C14	0.035 (3)	0.048 (3)	0.043 (3)	0.003 (2)	0.016 (2)	0.005 (2)
C15	0.044 (3)	0.047 (3)	0.036 (2)	0.017 (2)	0.017 (2)	0.003 (2)
C16	0.053 (3)	0.031 (3)	0.044 (3)	0.005 (2)	0.009 (2)	0.006 (2)
C17	0.042 (3)	0.034 (3)	0.039 (3)	0.003 (2)	0.009 (2)	0.001 (2)
C18	0.051 (3)	0.049 (3)	0.046 (3)	0.015 (3)	0.011 (3)	0.002 (3)
C19	0.043 (3)	0.038 (3)	0.042 (3)	−0.007 (2)	0.026 (2)	−0.007 (2)
C20	0.048 (3)	0.036 (3)	0.046 (3)	−0.009 (2)	0.022 (2)	−0.007 (2)
C21	0.036 (2)	0.040 (3)	0.034 (2)	0.010 (2)	0.014 (2)	0.003 (2)
C22	0.048 (3)	0.044 (3)	0.055 (3)	−0.005 (2)	0.032 (3)	−0.002 (2)
C23	0.046 (3)	0.036 (3)	0.055 (3)	−0.007 (2)	0.030 (3)	−0.005 (2)
C24	0.049 (3)	0.052 (3)	0.041 (3)	0.008 (3)	0.022 (2)	0.001 (2)
C25	0.076 (4)	0.044 (4)	0.077 (4)	−0.003 (3)	0.050 (4)	0.002 (3)
C26	0.047 (3)	0.044 (3)	0.073 (4)	−0.007 (3)	0.024 (3)	−0.002 (3)

Geometric parameters (Å, º)

Pd—N1	2.027 (4)	C2—H2	0.9500
Pd—N3	2.031 (4)	C3—C4	1.388 (7)
Pd—N5	2.029 (4)	C3—C6	1.437 (7)
Pd—N7	2.027 (4)	C4—C5	1.373 (7)
S1—O3	1.430 (4)	C4—H4	0.9500

S1—O1	1.434 (4)	C5—H5	0.9500
S1—O2	1.435 (4)	C7—C8	1.377 (7)
S1—C25	1.808 (6)	C7—H7	0.9500
S2—O4	1.433 (4)	C8—C9	1.383 (7)
S2—O5	1.438 (4)	C8—H8	0.9500
S2—O6	1.439 (4)	C9—C10	1.372 (7)
S2—C26	1.815 (6)	C9—C12	1.465 (7)
F1—C25	1.338 (8)	C10—C11	1.392 (6)
F2—C25	1.313 (7)	C10—H10	0.9500
F3—C25	1.325 (7)	C11—H11	0.9500
F4—C26	1.325 (7)	C13—C14	1.366 (7)
F5—C26	1.304 (7)	C13—H13	0.9500
F6—C26	1.335 (7)	C14—C15	1.393 (7)
N1—C5	1.344 (6)	C14—H14	0.9500
N1—C1	1.345 (6)	C15—C16	1.377 (7)
N2—C6	1.137 (7)	C15—C18	1.439 (7)
N3—C11	1.327 (6)	C16—C17	1.379 (7)
N3—C7	1.346 (6)	C16—H16	0.9500
N4—C12	1.135 (7)	C17—H17	0.9500
N5—C13	1.343 (6)	C19—C20	1.373 (7)
N5—C17	1.347 (6)	C19—H19	0.9500
N6—C18	1.146 (7)	C20—C21	1.385 (7)
N7—C23	1.330 (6)	C20—H20	0.9500
N7—C19	1.342 (6)	C21—C22	1.376 (7)
N8—C24	1.140 (6)	C21—C24	1.447 (7)
C1—C2	1.379 (6)	C22—C23	1.377 (7)
C1—H1	0.9500	C22—H22	0.9500
C2—C3	1.380 (7)	C23—H23	0.9500

N1—Pd—N7	87.80 (14)	C10—C9—C12	118.8 (5)
N1—Pd—N5	178.15 (15)	C8—C9—C12	121.1 (4)
N7—Pd—N5	90.70 (14)	C9—C10—C11	118.0 (5)
N1—Pd—N3	92.21 (14)	C9—C10—H10	121.0
N7—Pd—N3	179.53 (15)	C11—C10—H10	121.0
N5—Pd—N3	89.29 (14)	N3—C11—C10	122.4 (4)
O3—S1—O1	116.1 (3)	N3—C11—H11	118.8
O3—S1—O2	115.4 (3)	C10—C11—H11	118.8
O1—S1—O2	113.0 (2)	N4—C12—C9	179.4 (7)
O3—S1—C25	103.2 (3)	N5—C13—C14	122.4 (5)
O1—S1—C25	103.9 (3)	N5—C13—H13	118.8
O2—S1—C25	102.9 (3)	C14—C13—H13	118.8
O4—S2—O5	114.7 (3)	C13—C14—C15	118.5 (5)
O4—S2—O6	115.7 (3)	C13—C14—H14	120.8
O5—S2—O6	113.4 (2)	C15—C14—H14	120.8
O4—S2—C26	103.9 (3)	C16—C15—C14	119.4 (5)
O5—S2—C26	102.8 (2)	C16—C15—C18	120.5 (5)
O6—S2—C26	104.2 (3)	C14—C15—C18	120.1 (5)
C5—N1—C1	119.0 (4)	C15—C16—C17	119.2 (5)

C5—N1—Pd	121.6 (3)	C15—C16—H16	120.4
C1—N1—Pd	119.3 (3)	C17—C16—H16	120.4
C11—N3—C7	119.1 (4)	N5—C17—C16	121.3 (5)
C11—N3—Pd	120.7 (3)	N5—C17—H17	119.4
C7—N3—Pd	120.2 (3)	C16—C17—H17	119.4
C13—N5—C17	119.2 (4)	N6—C18—C15	179.0 (6)
C13—N5—Pd	119.8 (3)	N7—C19—C20	121.7 (4)
C17—N5—Pd	121.0 (3)	N7—C19—H19	119.1
C23—N7—C19	119.3 (4)	C20—C19—H19	119.1
C23—N7—Pd	120.2 (3)	C19—C20—C21	118.6 (5)
C19—N7—Pd	120.4 (3)	C19—C20—H20	120.7
N1—C1—C2	122.0 (4)	C21—C20—H20	120.7
N1—C1—H1	119.0	C22—C21—C20	119.7 (4)
C2—C1—H1	119.0	C22—C21—C24	121.3 (5)
C1—C2—C3	118.8 (5)	C20—C21—C24	119.1 (5)
C1—C2—H2	120.6	C21—C22—C23	118.3 (5)
C3—C2—H2	120.6	C21—C22—H22	120.8
C2—C3—C4	119.2 (4)	C23—C22—H22	120.8
C2—C3—C6	120.0 (5)	N7—C23—C22	122.3 (5)
C4—C3—C6	120.8 (5)	N7—C23—H23	118.8
C5—C4—C3	119.0 (5)	C22—C23—H23	118.8
C5—C4—H4	120.5	N8—C24—C21	179.4 (6)
C3—C4—H4	120.5	F2—C25—F3	107.5 (5)
N1—C5—C4	122.0 (5)	F2—C25—F1	106.5 (6)
N1—C5—H5	119.0	F3—C25—F1	108.1 (5)
C4—C5—H5	119.0	F2—C25—S1	112.5 (4)
N2—C6—C3	178.1 (7)	F3—C25—S1	111.7 (4)
N3—C7—C8	121.9 (5)	F1—C25—S1	110.2 (4)
N3—C7—H7	119.0	F5—C26—F4	107.6 (5)
C8—C7—H7	119.0	F5—C26—F6	106.6 (5)
C7—C8—C9	118.5 (5)	F4—C26—F6	107.5 (5)
C7—C8—H8	120.8	F5—C26—S2	112.4 (4)
C9—C8—H8	120.8	F4—C26—S2	112.2 (4)
C10—C9—C8	120.1 (4)	F6—C26—S2	110.3 (4)

N7—Pd—N1—C5	105.2 (3)	Pd—N5—C13—C14	178.3 (4)
N3—Pd—N1—C5	−74.3 (3)	N5—C13—C14—C15	−0.7 (7)
N7—Pd—N1—C1	−70.1 (3)	C13—C14—C15—C16	0.9 (7)
N3—Pd—N1—C1	110.4 (3)	C13—C14—C15—C18	−179.2 (5)
N1—Pd—N3—C11	115.5 (4)	C14—C15—C16—C17	−0.2 (7)
N5—Pd—N3—C11	−65.6 (4)	C18—C15—C16—C17	179.9 (5)
N1—Pd—N3—C7	−67.5 (3)	C13—N5—C17—C16	0.9 (7)
N5—Pd—N3—C7	111.5 (3)	Pd—N5—C17—C16	−177.5 (4)
N7—Pd—N5—C13	81.3 (3)	C15—C16—C17—N5	−0.7 (8)
N3—Pd—N5—C13	−99.2 (3)	C23—N7—C19—C20	0.1 (7)
N7—Pd—N5—C17	−100.3 (4)	Pd—N7—C19—C20	−176.4 (4)
N3—Pd—N5—C17	79.2 (4)	N7—C19—C20—C21	0.0 (7)
N1—Pd—N7—C23	−88.8 (4)	C19—C20—C21—C22	−0.4 (7)

N5—Pd—N7—C23	92.3 (4)	C19—C20—C21—C24	178.8 (5)
N1—Pd—N7—C19	87.7 (4)	C20—C21—C22—C23	0.7 (7)
N5—Pd—N7—C19	−91.3 (4)	C24—C21—C22—C23	−178.5 (5)
C5—N1—C1—C2	−1.2 (7)	C19—N7—C23—C22	0.2 (7)
Pd—N1—C1—C2	174.3 (3)	Pd—N7—C23—C22	176.7 (4)
N1—C1—C2—C3	−0.5 (7)	C21—C22—C23—N7	−0.6 (8)
C1—C2—C3—C4	1.6 (7)	O3—S1—C25—F2	−62.4 (6)
C1—C2—C3—C6	−177.7 (5)	O1—S1—C25—F2	59.2 (6)
C2—C3—C4—C5	−1.1 (7)	O2—S1—C25—F2	177.3 (5)
C6—C3—C4—C5	178.2 (4)	O3—S1—C25—F3	58.7 (5)
C1—N1—C5—C4	1.7 (7)	O1—S1—C25—F3	−179.7 (4)
Pd—N1—C5—C4	−173.6 (3)	O2—S1—C25—F3	−61.6 (5)
C3—C4—C5—N1	−0.6 (7)	O3—S1—C25—F1	178.8 (4)
C11—N3—C7—C8	0.7 (7)	O1—S1—C25—F1	−59.5 (5)
Pd—N3—C7—C8	−176.3 (4)	O2—S1—C25—F1	58.5 (5)
N3—C7—C8—C9	0.2 (7)	O4—S2—C26—F5	−65.3 (5)
C7—C8—C9—C10	−0.9 (7)	O5—S2—C26—F5	174.8 (5)
C7—C8—C9—C12	177.8 (5)	O6—S2—C26—F5	56.3 (5)
C8—C9—C10—C11	0.6 (7)	O4—S2—C26—F4	56.1 (5)
C12—C9—C10—C11	−178.0 (4)	O5—S2—C26—F4	−63.8 (5)
C7—N3—C11—C10	−1.0 (7)	O6—S2—C26—F4	177.7 (4)
Pd—N3—C11—C10	176.1 (3)	O4—S2—C26—F6	175.9 (4)
C9—C10—C11—N3	0.3 (7)	O5—S2—C26—F6	56.0 (5)
C17—N5—C13—C14	−0.2 (7)	O6—S2—C26—F6	−62.5 (5)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···N8^{i}	0.95	2.56	3.489 (8)	166
C5—H5···O2	0.95	2.44	3.159 (6)	132
C7—H7···O5^{ii}	0.95	2.52	3.202 (6)	129
C8—H8···N6^{iii}	0.95	2.53	3.441 (8)	160
C13—H13···O5^{ii}	0.95	2.33	3.134 (7)	141
C16—H16···N6^{iv}	0.95	2.61	3.403 (8)	142
C22—H22···O3^{v}	0.95	2.52	3.170 (7)	126
C23—H23···O2	0.95	2.34	3.163 (7)	145

Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+3/2; (ii) *x*, *y*−1, *z*; (iii) −*x*, *y*−1/2, −*z*+3/2; (iv) −*x*, −*y*+1, −*z*+1; (v) −*x*+1, *y*−1/2, −*z*+3/2.